IV. Regional Model Estimates of USBO, Reconciling observations and models and uncertainties (Gail, 2,000 words)

Summary of how models are used in the regulatory context: SIPs/TIPs, model attainment demonstrations, relative response factors and selection of days to analyze for RRF. Describe typical model performance evaluations (MPE) in regulatory context, and provide examples of applications that have benefited from intensive field studies (TEXAQS).

Brief summary of O3 chemistry and modeled sensitivity to VOC and NOx.

Key uncertainties:

- Do models accurately simulate relative contributions of transported O3 versus locally produced O3. Describe use of rural monitoring to evaluate regional scale model performance.
- Do models accurately simulate model response to VOC and NOx. Summarize dynamic model evaluations studies.
- Do the MOVES model and the NEI accurately represent VOC and NOx emissions?
- Effects of uncertainty in biogenic and lightning NOx.
- Do models accurately simulate the fate and recycling of reactive NOx? What studies are needed to evaluate partitioning of NOx into organic nitrates, PANs and HNO3.

Should we summarize regional difference in model uncertainty and needs for model evaluation?

Northeastern states: Uncertainty in mobile source NOx emissions; long range transport from upwind states.

Southeastern states: larger contribution of biogenic VOC and more NOx limiting conditions.

Midwest: transport over great lakes; contribution to downwind states.

Western states: larger contributions from background sources, including wildfires, international transport and stratospheric intrusion; high elevation and deeper PBL, increasing energy development.

Draft Text on Regional Models

Photochemical grid models have been widely used in the air quality planning and regulatory community since the 1980s (Tesche et al., 199x). Comprehensive reviews of early photochemical modeling applications include Seinfeld (1988), NRC (1991) and Russell and Dennis (2001). Early regulatory modeling efforts relied on urban scale model domains to simulate episodes of several days using static boundary conditions that were based on observed O3 mixing ratios. This approach was appropriate for conditions in which urban O3 levels could exceed 200 ppb and for which O3 was mostly produced from local precursor emissions during stagnation episodes that lasted for a few days. Beginning in the 2000s, with increasing interest in the effects of O3 deposition on vegetation and the role of O3 in reactions that form secondary fine particulates, high resolution national scale models were developed to simulate O3 in rural and remote areas for annual simulation periods. With regional haze modeling studies, it was recognized that global transport is an important source of intraday variability and spatial variability in both O3 and PM2.5, and regulatory modeling studies began to use global model simulations to provide time and spatially varying BC data for higher resolution regional and urban scale model simulations (Morris et al.200x). Moreover, there have been large reductions in urban precursor emissions and ambient O3 levels since the 1980s, while the level of the NAAQS has been reduced from a one hour average of 120 ppb to an 8 hour average of 70 ppb. As a result, USBO now contributes a greater proportion of ambient O3 in non-attainment areas, and there is increased emphasis on accurately simulating day specific contributions of USBO to exceedances of the NAAQS (references WAQS, Texas modeling?).

Recent regulatory photochemical modeling studies have used both the Comprehensive Air Quality Model with extensions (CAMx, ENVIRON, 201x) and the Community Multiscale Air Quality Model (CMAQ, EPA, 201x). Both models have similar science algorithms for chemistry, transport and removal of pollutants, and both require input data from the Weather Research and Forecasting (WRF) model and emissions inventory data that is processed using the SMOKE. The WRF-Chem model has been used extensively in air quality research studies (reference, UBOS, fire papers) but is not typically used for regulatory studies.

Areas that violate the O3 NAAQS are required to develop a state implementation plan (SIP) that describes measures adopted to bring the area into compliance with the NAAQS. For areas that exceed the O3 NAAQS with a marginal classification, photochemical modeling is not required in the planning process because it is presumed that these areas will attain the NAAQS as a result of national control measures such as reduced vehicle emissions and cleaner fuels. For areas that exceed the O3 NAAQS with a classification of moderate or greater, states are required to develop a model attainment demonstration that includes emissions reductions sufficient to achieve the NAAQS by a specific date (cite EPA Rule/Guidance). Additionally, upwind states that may contribute to O3 NAAQS violations are required to assess their contributions to the violating monitor, and photochemical models may also be used to evaluate interstate transport. The modeling system (including WRF, CMAQ or CAMx, and SMOKE) is evaluated for an historical O3 episode, and if the model performs sufficiently well, it is then applied with emissions reductions for a future year scenario to assess whether planned emissions reductions are adequate to achieve the O3 NAAQS. EPA Guidance for model evaluation (EPA, 2014) explains the types of analyses that should be completed as part the of model performance evaluation (MPE). Because models are subject to bias an error when simulating ambient O3, absolute models results are not used to assess compliance with planning requirements. Instead, model relative response factors (RRF) are used to evaluate the modeled percent reduction in the future attainment year, and the RRF is applied to the baseline O3 design value to evaluate compliance.

The Colorado SIP (Colorado Air Quality Control Commission, 2016) can be used to illustrate the effects uncertainty off model uncertainty in estimates of USBO. The Colorado Regional Air Quality Council (RAQC) selected summer of 2011 for their attainment demonstration base case MPE. The WRF and CAMx modeling platform used a high resolution 4-km grid for the state of Colorado that was nested within western U.S. 12-km grid, and 36-km North America CAMx simulations developed by the Western Air Quality Study (WAQS, reference). Day specific boundary conditions for the 36-km CAMx simulation were derived from a 2011 simulation of the MOSART model (reference). Emission data are described by the Colorado Department of Public health (CDPHE 2016a, 2016b, 2016c). The WRF and CAMx configuration and MPE are described in Ramboll-Environ (2016) who used both quantitative (model performance statistics) and qualitative (graphical displays) MPE approaches. For the 4 key monitoring sites in the Denver NAA, they found that the model achieved typical performance goals bias ranging from -7% to –11% for all hours with observed O3 greater than 60 ppb. Focusing on the Chatfield monitor which has the highest O3 levels, the model was biased low in May and June and biased high in July and August. While the model achieved the performance goal, it failed to accurately simulate the days with the highest monitored O3. Table X list the highest modeled and monitored days at the Chatfield site in 2011. Only one of the highest 10 monitored days (8/27/2011) was included among the highest 10 modeled days, and the model was biased on many of the highest modeled days.

Spatial plots of the modeled and observed O3 values can provide valuable insight into the causes of poor model performance, and in this case, can identify three ways in which the model can perform poorly in Colorado. Figure X-a shows the observed and modeled on June 7th, the second highest observed O3 day with an 8-hour average of 84 ppb at the Chatfield monitor. The monitoring data show an extensive region of elevated O3 in rural and urban central Colorado at 10 am local time. The large spatial extent, including rural area early in the day indicated the high O3 levels are caused by transport rather than local photochemical production. While the model does simulate enhanced O3 in the range of 60 to 70 ppb in central Colorado, it is biased low by as much as 20 ppb compared to rural sites west of Denver. Figure X-b shows observed and modeled O3 for July 5th, the highest modeled day with an MD8 of 84 ppb, but with positive bias of 21% and an observed MD8 of 69 ppb. The model had large positive bias, from 10to 20 ppb, at rural sites throughout Colorado on this day, indicating that the model may have overestimated USBO on this day. Figure X-c shows observed and modeled O3 for July 18th, the 7th highest observed day with an MD8 of 79 ppb. While the model successfully predict rapid photochemical production of O3 in the Denver area on this day, the WRF meteorological fields appear to transport the O3 too rapidly into the foothills west of the Denver area. As a result, the model is biased low at the Chatfield monitor and this day is not among the highest modeled O3 days.

Bias in model performance for urban O3 and USBO can affect the Colorado SIP attainment demonstration in several ways. Table X also shows the 2017 modeled MD8 at the Chatfield monitor for the highest modeled days, and the RRF, the ratio of the modeled MD8 in 2017 to 2011. While Colorado reduced modeled precursor emissions by 30% from 2011 to 2017, the 2017 modeled O3 is reduced by 3 to 8% on the highest days. For July 5th, one of the days one which the model appears to overestimate USBO, modeled O3 is reduced by only 5% in 2017. If the model overestimates USBO and underestimates local production of O3, the model will also underestimate the benefits of reducing local precursor emissions. While there have been limited long term dynamic model evaluation studies, there is evidence to suggest that models have underestimated the effectives of precursor reductions, and this could be a result of models that overestimate USBO. The model can also underestimate the benefits of local precursor reduction if it fail to accurately simulate the transport of locally produce O3, as shown in Figure X-c for July 18th. Alternatively, the model can overestimate the benefits of precursor emissions reductions if it underestimates USBO on days with high O3 levels, as was shown in Figure X-a for June 7th. The Exceptional Events rule is intended to exclude certain days with high USBO from the evaluation of the compliance with the NAAQS, but if these days are not successfully identified and excluded, states could fail to achieve the expected progress towards compliances with the NAAQS. The rural monitoring data in Colorado indicated that several of the highest 10 observed O3 days in June 2011, listed in Table X, may have been influenced by long range transport of O3, but these days were not flagged or excluded under the EE Rule.

Source attribution Approaches in Regional Models.

The objective of source attribution techniques is to provide quantitative estimates of the source categories that contribute to O3. A simple and frequently used approach is to perform model sensitivity simulations for a base case and a sensitivity case with a source category removed from the model, and source contributions are evaluated by comparing the two simulations. Sensitivity approaches can be computationally expensive because a new model simulation is required for each sensitivity parameter, and interpretation of results can be complex because of non-linear processes in the model. Other source attributions approaches have been developed to reduce computation cost and to address non-linearity in the model, and these include source apportionment techniques that use reactive tracer species (Ramboll-Environ, 2016; Kwok et al., 2015), the Decoupled Direct Method (DDM, Dunker et al.,2002) and backward (adjoint) methods (Mesbah et al., 2012). Kwok et al. (2015) review and discuss benefits of each of these approaches.

Conceptually, the simplest modeling approach to estimate USBO is to perform a model simulation that includes all natural sources of O3 within the U.S., including biogenic and geogenic precursors, but to exclude ("zero-out") all U.S. anthropogenic precursors. For regional scale models, this approach also requires BC data derived from a global CTM simulation that includes international anthropogenic emissions but excludes U.S. anthropogenic emissions (e.g., Henderson et al., 2014). Dolwick et al. (2015) compared USBO estimates using CMAQ zero-out and CAMx source apportionment approaches in regional model simulations using a 12-km grid for 2007. The 2007 CMAQ and CAMx simulations estimated that seasonal mean USBO MDA8 O3 levels ranged from 25-50 ppb across the U.S. Locations with seasonal mean contributions greater than 40 ppb are confined to the inter-mountain western U.S., with substantially lower values in the eastern U.S. and along the Pacific Coast, and USBO was estimated to represent a relatively larger percentage (e.g., 60-80%) of the seasonal mean total MDA8 O3 at locations within the inter-mountain western U.S. and along the U.S. borders with Mexico and Canada. Dolwick et al. (2015) found that the CMAQ zero-out and CAMx source apportionment approaches estimated similar USBO impacts over the rural areas, but the CAMx source apportionment approach predicted lower USBO contributions in urban areas because anthropogenic emissions react with and destroy some fraction of the ozone in the CAMx tracer species used to track the background ozone contribution.

A limitation of the Dolwick et al. (2015) study is that it evaluated typical USBO levels across the western U.S. for 2007 using climatological monthly-average wildfire and typical-day major point source emissions but was not intended to capture discrete high O3 events that occurred in 2007. In contrast, WAQS modeling for 2011 used day specific modeling emissions estimates, using both the CAMx and CMAQ models with a 12-km grid for the western U.S and a 4-km grid for intermountain states. CAMx source apportionment simulations were used to estimate background contribution from international transport and biogenic U.S. emissions, including wildfires. BC data were derived from the MOZART model, and additional CAMx simulations were performed using BC data from the GEOS-Chem and AM3 models. All of the global model simulations included U.S. anthropogenic emissions, thus the BC include O3 from U.S. emissions that circle the globe and are not directly comparable other estimates of USBO. In addition to the CAMx source apportionment simulations, the WAQS performed U.S. anthropogenic zero-out sensitivity simulations to estimate background O3 levels.

Summary of CAMx OSAT/APCA results.

Comparison of APCA to zero-out result.

There is uncertainty in model estimates of USBO for days on which the model has large bias or error in simulating regional O3 levels. The O3 spatial plots in Figure X identify specific days on which the WAQS and Denver SIP models performed poorly for regional O3 and for a high background O3 day on June. Additional spatial plots available at the WAQS (reference) show that the model is frequently biased low for what appear to be regional scale O3 transport events in May and June. More comprehensive MPE studies are need to identify the causes of poor model performance on these days and to evaluate how this affects model estimates of USBO.

A limitation of previous USBO regional modeling studies is that the BC data from global CTM have not preserved source attribution data for O3 transported into the regional model. Thus, the regional model studies were not able to distinguish contributions to O3 from natural precursors, international anthropogenic precursors, and the stratosphere. Future modeling studies designed to evaluate international anthropogenic contributions will required that global CTM include O3 source attribution estimates for anthropogenic, natural and stratospheric O3, and BC data derived from the global models should include this data so that it can be passed to and tracked within the regional models.

Additional References

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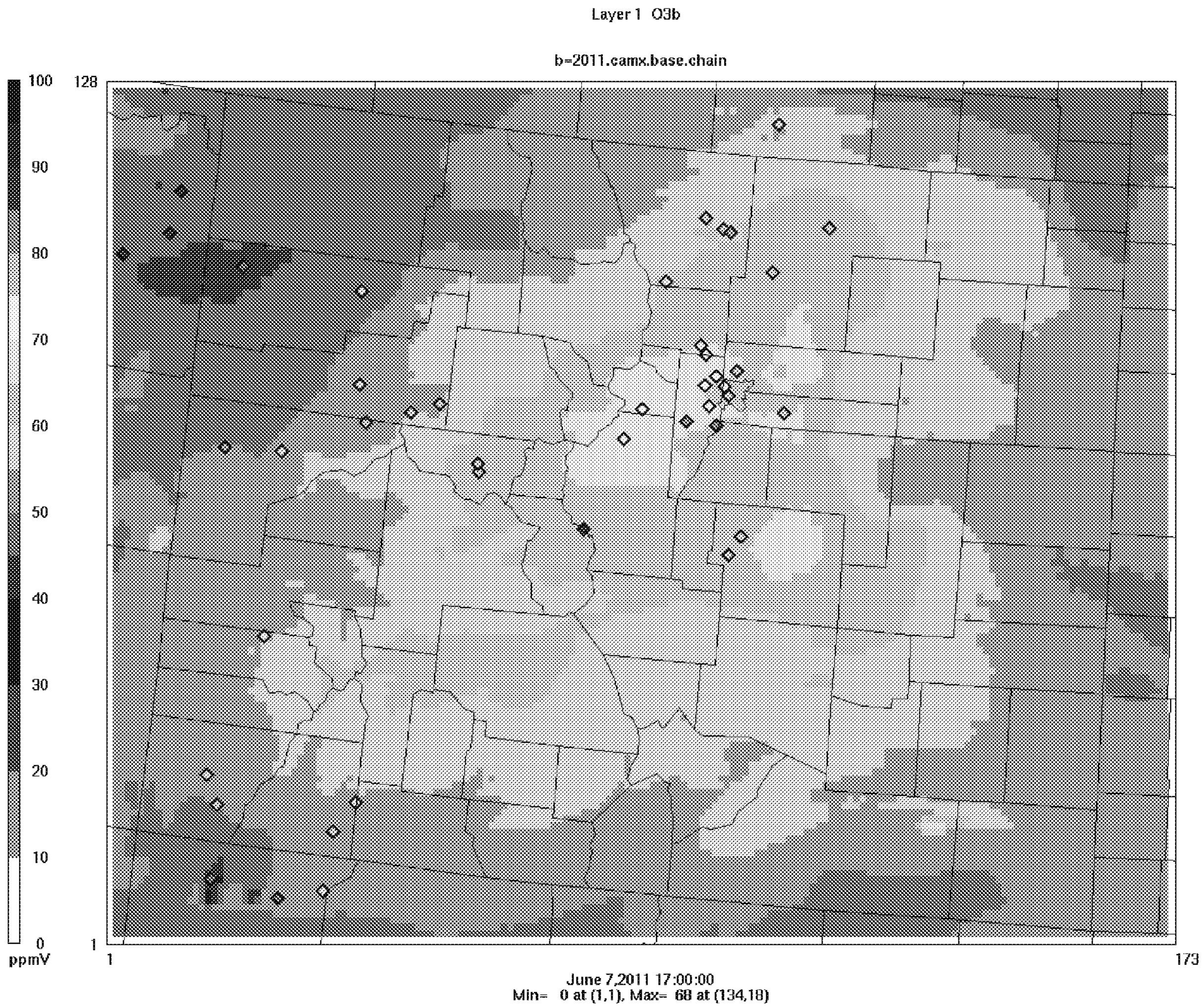
Figure . Colorado SIP 4-km CAMx model domain, nested within the WAQS 12-km and 36-km domains, with boundary condition data for the 36-km domain derived from the MOZART global chemistry transport model.

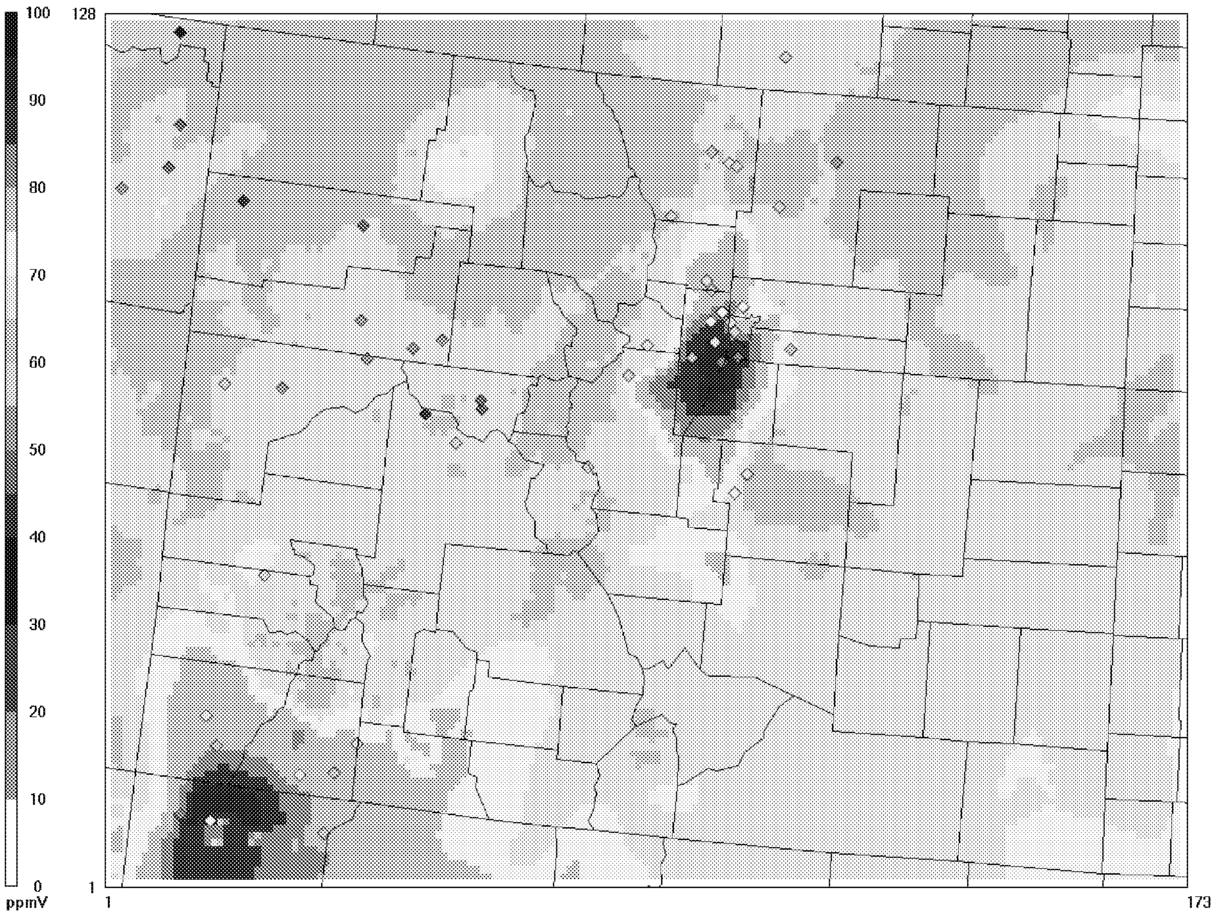
Table X. Highest ten modeled and observed O3 days at the Chatfield monitor.

Highest 10 modeled O3 days						Highest 10 observed O3 days	
Date	2011 Observed	2011 Model	Bias%	2017 Model	RRF 2017/2011	Date	2011 Observed
7/5/2011	69	84	21%	79	0.95	6/24/2011	99
7/12/2011	71	83	17%	78	0.93	6/7/2011	84
8/26/2011	71	83	17%	77	0.93	8/13/2011	84
7/4/2011	63	81	30%	77	0.94	8/12/2011	82
8/3/2011	67	81	21%	75	0.93	8/20/2011	81
7/6/2011	71	80	12%	78	0.97	8/27/2011	81
8/27/2011	81	80	-1%	75	0.94	7/18/2011	79
7/23/2011	73	78	7%	75	0.95	7/30/2011	78
7/29/2011	66	78	18%	71	0.92	6/22/2011	76
8/22/2011	75	78	3%	73	0.93	8/23/2011	76



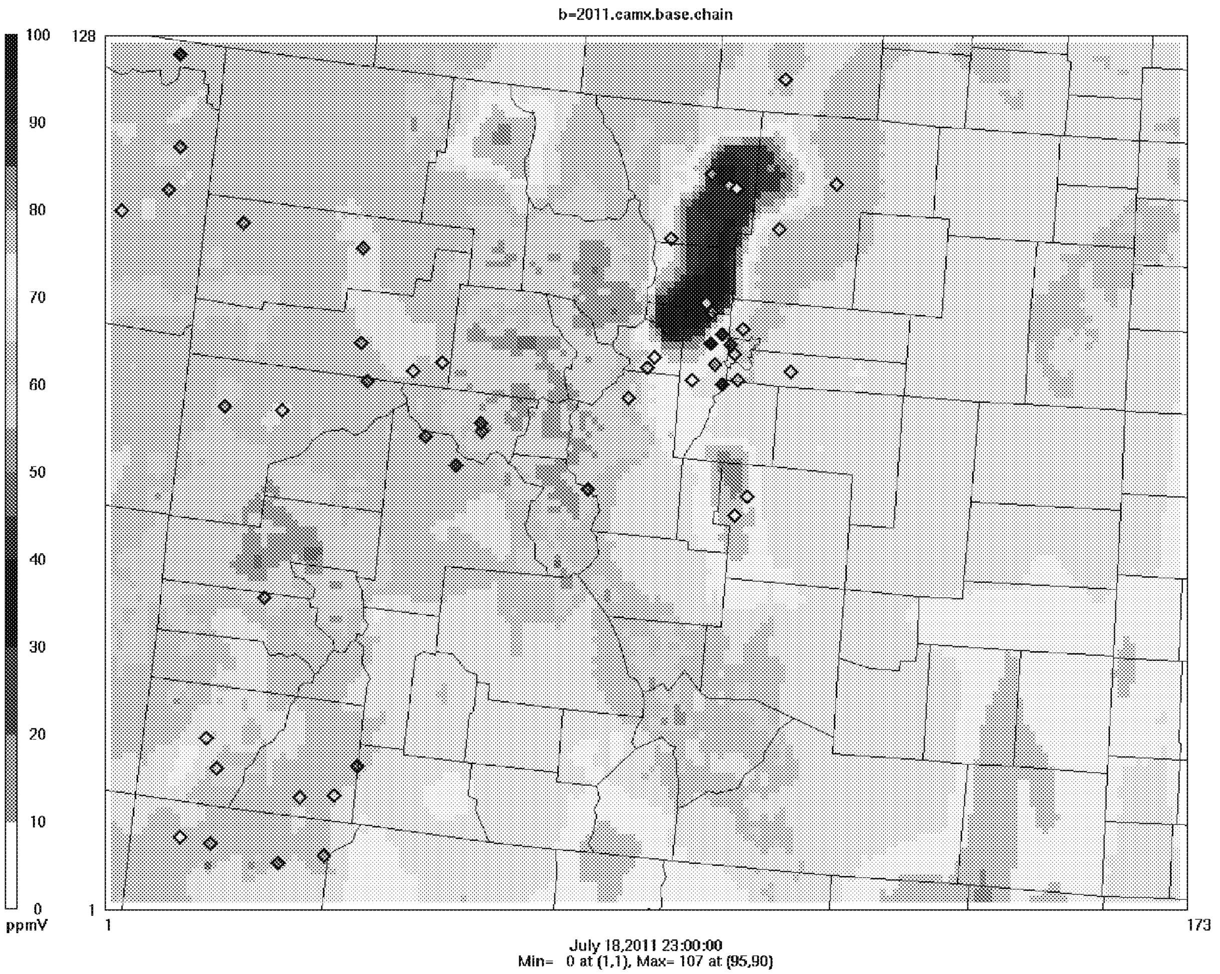
Layer 1 O3b

b=2011c.camx.base.chain



July 5,2011 20:00:00
Min= 0 at (1,1), Max= 95 at (17,13)

Layer 1 O3b



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